An Idea to Address Uncertainty in Mapping at the RI Stage of the LPR Project

ANCHOR
QEA

Meeting of CPG and EPA Region 2

January 27, 2016

Outline

- Introduction

- Overview of conditional simulation

- Application of conditional simulation
  - Illustrated with preliminary results

Maps of Sediment COC Concentrations are Basis for Crafting & Evaluating Remedial Alternatives

- Supported by an array of data
  - Contaminant concentrations
  - Sediment type
  - Bathymetry
  - Long-term erosion/deposition patterns

Maps Only Provide Estimates of the True Concentration Patterns

- On average have 0.5 samples per acre of river bottom

- Estimates at unsampled locations can have considerable error (uncertainty)

Uncertainty is Acceptable for FS

- Recognized and accepted fact at the FS stage of a CERCLA project

- Constrained by knowledge of the river

- Favorable test of map at RM 10.9

Surface-weighted Area Concentration Estimates for RM 10.9 Design Area

	Exclude Design Data	Include All Data
Cores per acre	0.9	7.7
Pre-remedial SWAC (ng/kg)	3,361	3,179
Post-remedial SWAC (ng/kg)	85	95
Percentage SWAC reduction	97%	97%
Target area (acres)	6.1	5.1
Non-target area (acres)	6.9	7.9
Net percent area change	—	7.3%
SWAC outside footprint (ng/kg)	159	157
SWAC within footprint (ng/kg)	7,022	7,835

But, CPG Recognizes Other Region 2 Concerns With CPG Thiessen Polygon Maps

- Magnitude of uncertainty outside of RM 10.9

- Possibility for high bias in estimates of remedy effectiveness

  – Overstating magnitude of high concentrations

  – Understating magnitude of low concentrations

To Quantify Uncertainty and Address Potential Bias, CPG Has Explored the Following

- Conditional simulation based on kriging to quantify uncertainty

Inspired by R2 White Paper & Approaches Used Elsewhere

- WP simulation illustrating uncertainty and bias issues

- Oil & gas and mining industries mapping of deposits

- EPA recommended method for characterizing wastes (EPA/600/R-92-033)

- EPA approach to target sampling to reduce uncertainty at East Poplar Creek & Lower Fox River

- EPA estimate uncertainty of contaminated sediment volume at Trenton Channel

- EPA crafting of remedial alternatives at Kalamazoo River

- GE and EPA evaluating exposure concentrations for the Hudson River floodplain

Proposed Uses of Conditional Simulation

- Develop 100 plausible maps of concentrations

- Use maps to support crafting remedial options
  - Based on the 100 estimates of concentration reduction associated with any remedial action level (RAL)

- Use maps to inform data collection during remedial design
  - Identify areas with greatest uncertainty relative to RAL and target with greatest sampling density

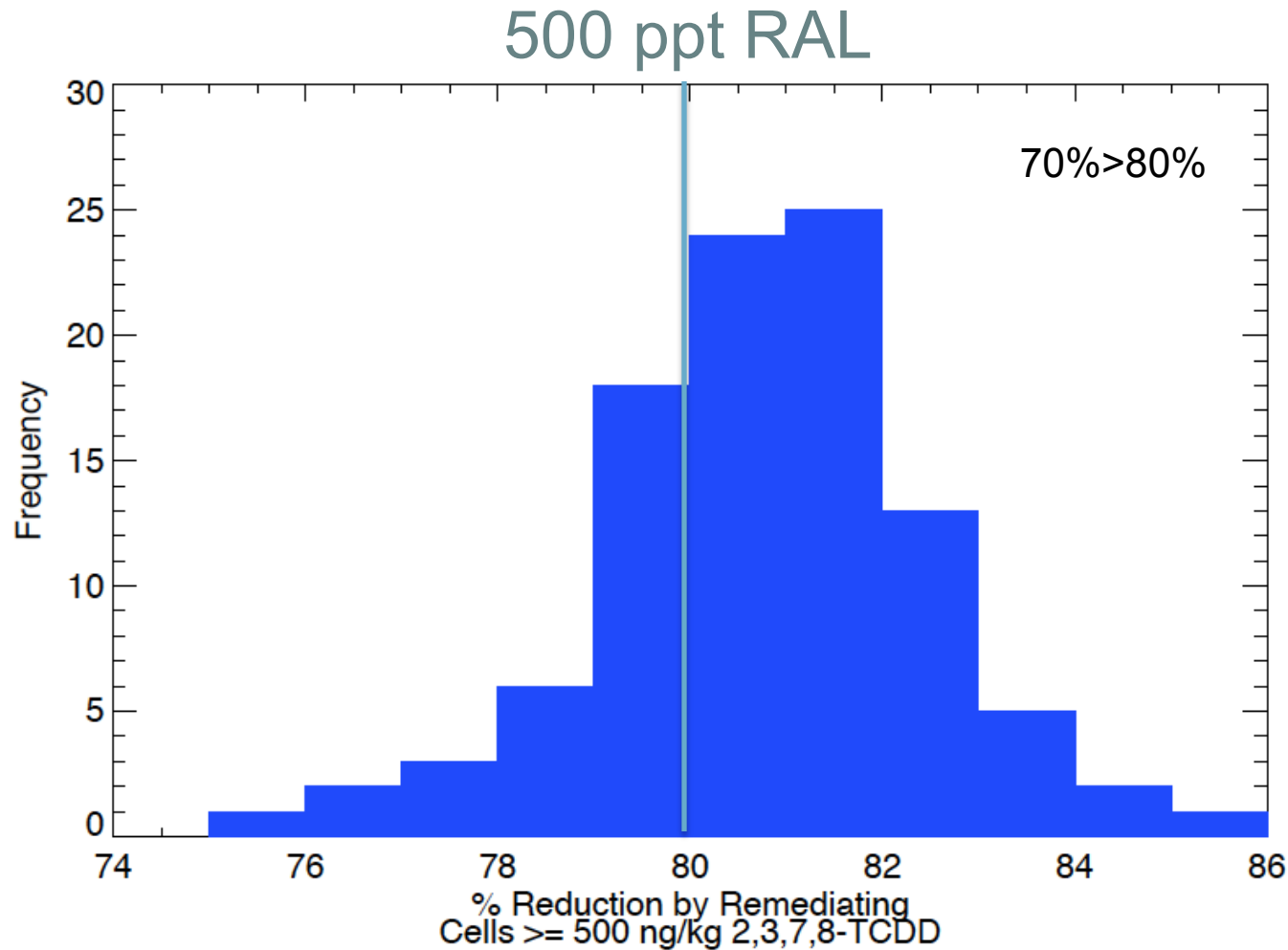# Use of Conditional Simulation to Craft Remedial Options for FS Evaluation

- Choosing an RAL
  - Could choose RAL that achieves greater than a specified reduction with a define level of confidence (e.g., 80% chance of achieving more than an 80% reduction)

- Choosing an area to target at a given RAL
  - Could choose conservative estimate of area meeting an RAL (e.g., 80% upper bound on area)

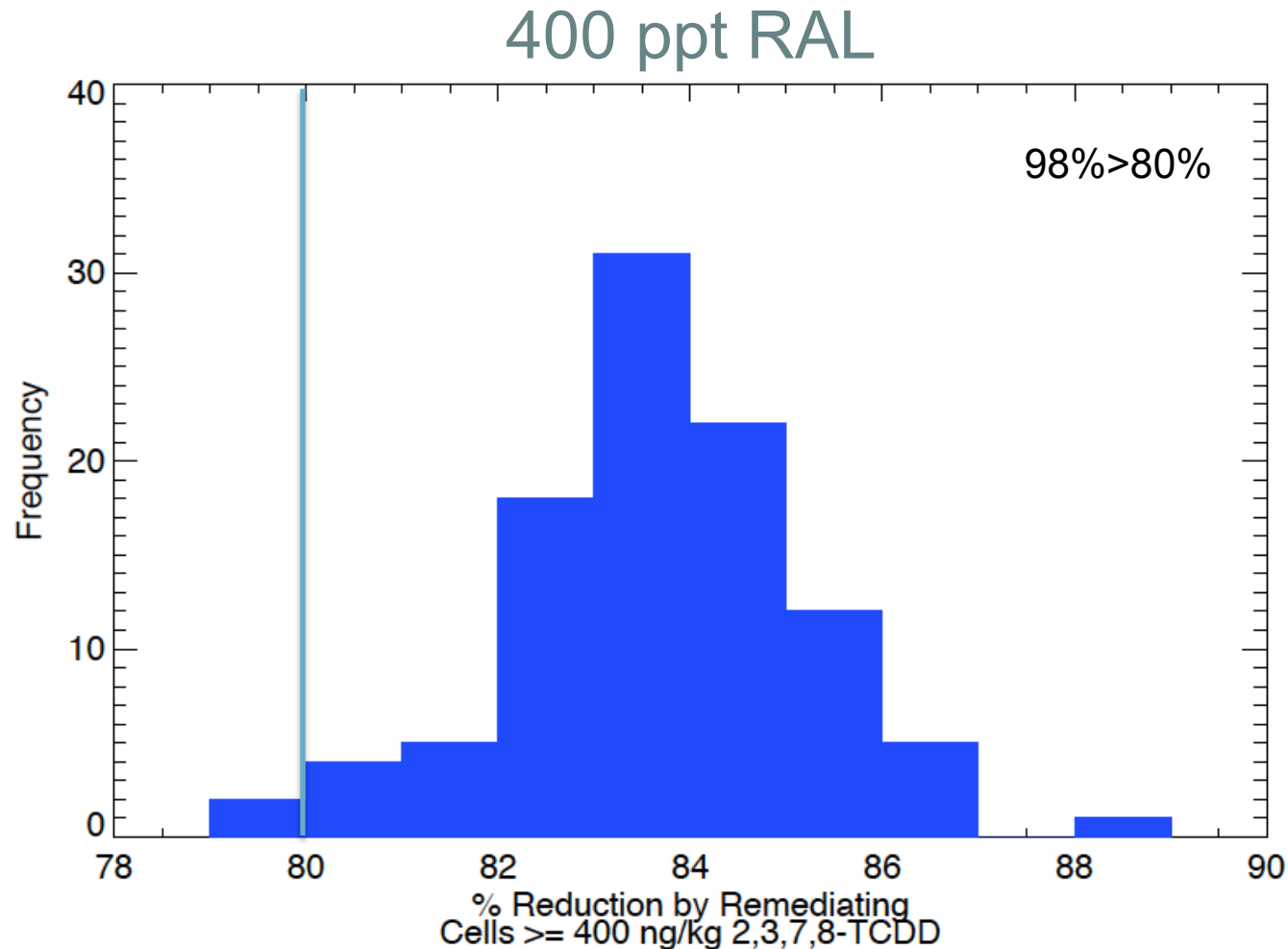*Results that follow to illustrate these ideas are based on CPG initial efforts that are subject to refinement*

Range of Possible Concentration Reductions Give Perspective on Uncertainty
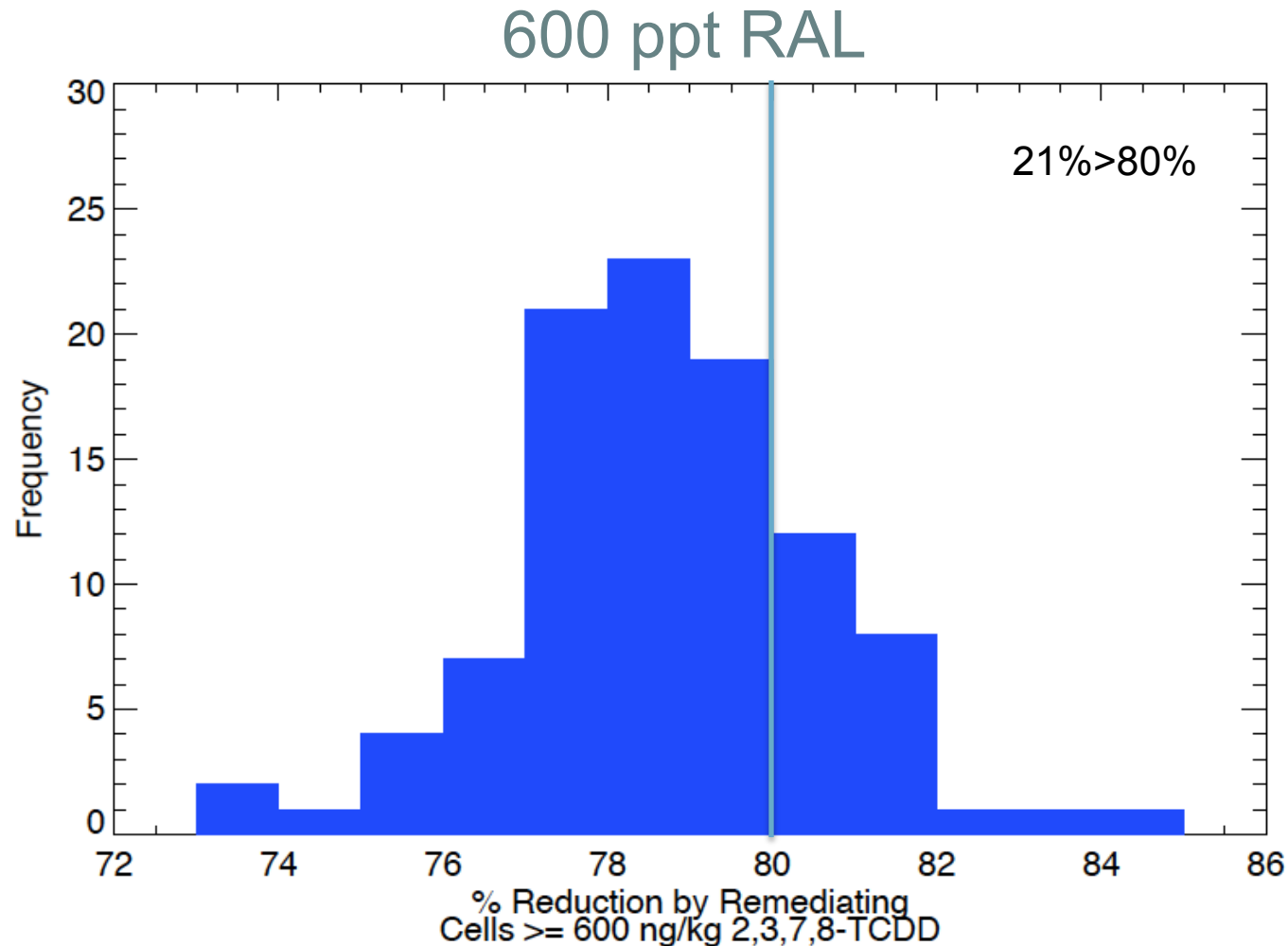
600 ppt RAL

21%>80%

% Reduction by Remediating
Cells >= 600 ng/kg 2,3,7,8-TCDD

Range of Possible Concentration Reductions Give Perspective on Uncertainty

500 ppt RAL

70%>80%

% Reduction by Remediating
Cells >= 500 ng/kg 2,3,7,8-TCDD

Range of Possible Concentration Reductions Give Perspective on Uncertainty

400 ppt RAL

Range of Possible Concentration Reductions Give Perspective on Uncertainty

Likelihood of >80% Reduction
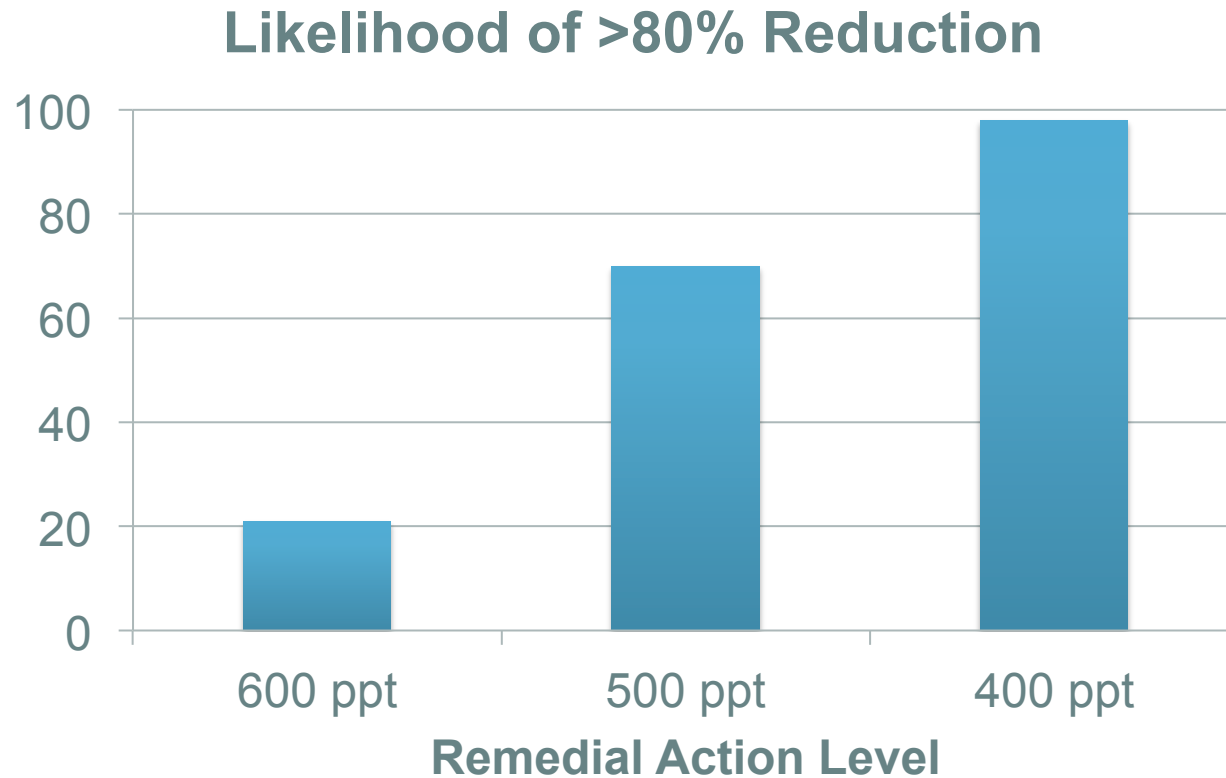
Uncertainty in Area Meeting an RAL Informs Choice of Area to Characterize a Remedial Option

500 ppt RAL

Upper 80th percentile is 193 acres
Upper 95th percentile is 200 acres

Note: CPG Thiessen Polygon map indicated 139 acres
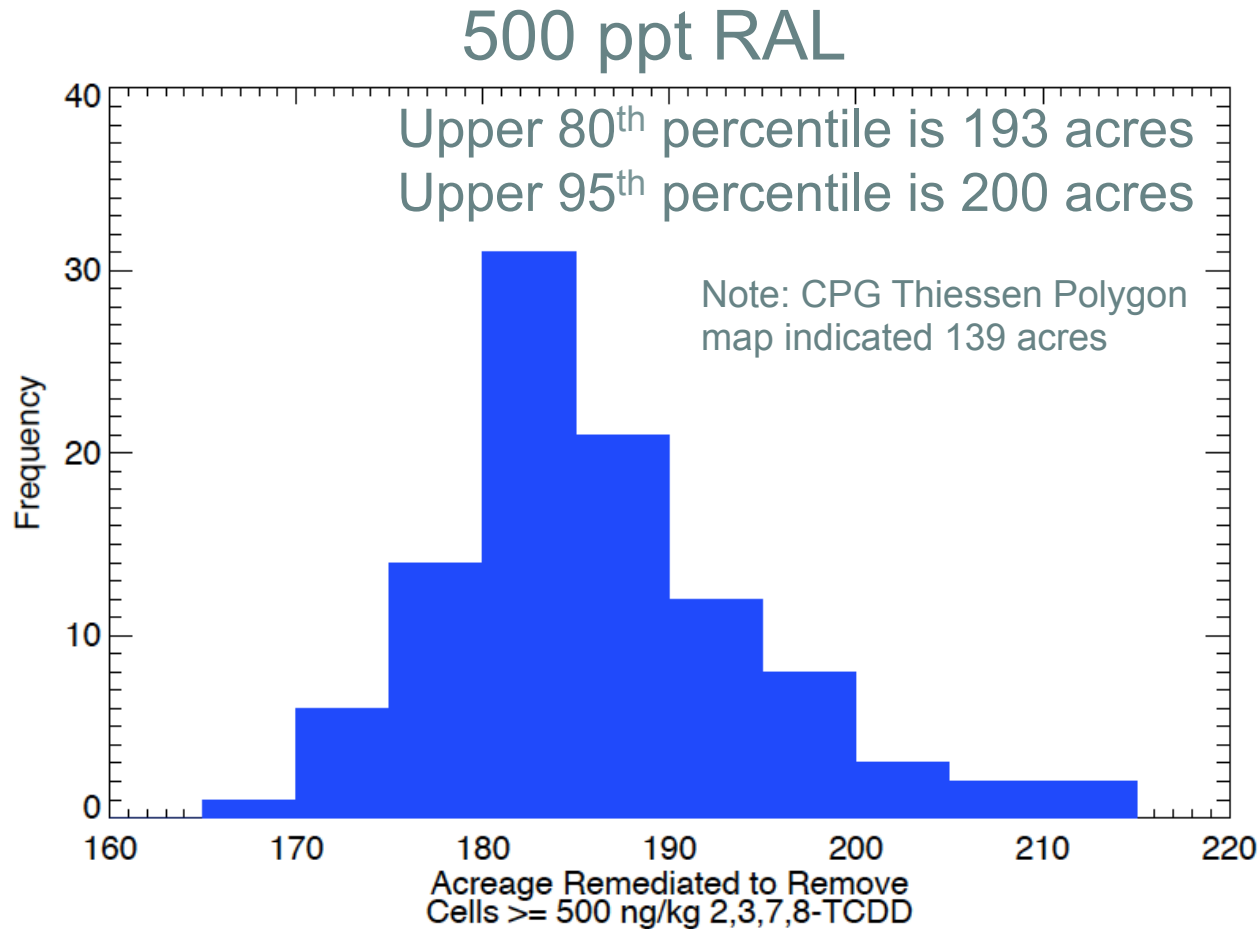
CS results can provide basis to focus design sampling

Greatest density in areas with greatest uncertainty about meeting an RAL (e.g., 33 to 66 percent chance – cyan & yellow in the figure)

RM 9.5

Interpolation Boundaries

Percentage >= 500 ng/kg
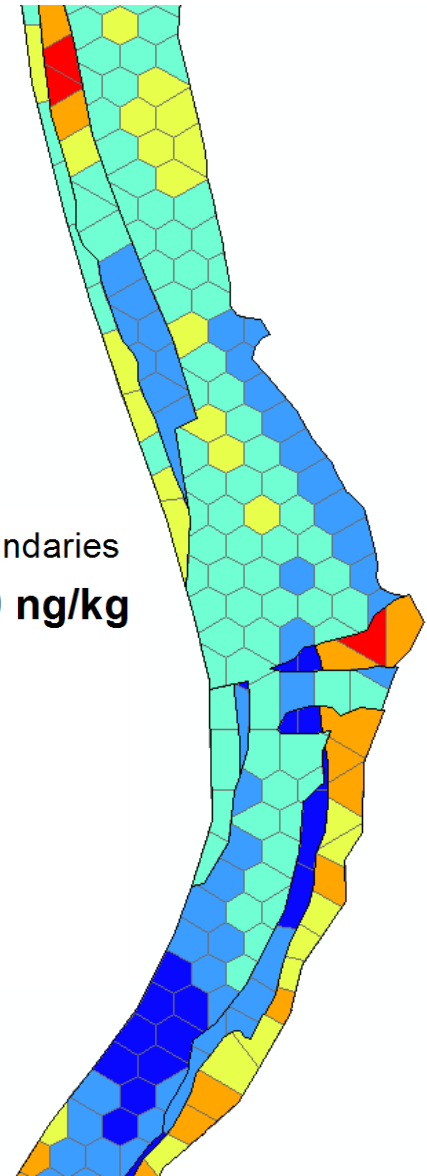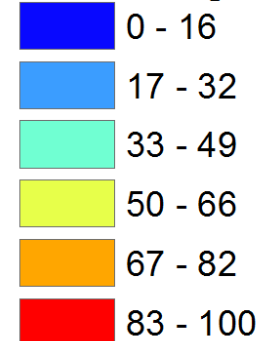
- 0 - 16
- 17 - 32
- 33 - 49
- 50 - 66
- 67 - 82
- 83 - 100

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Overview of Applied Geostatistical Approaches

- Kriging

  - Interpolate on fine grid using measured values and a model of spatial correlation (variogram)

  - Predict a distribution of possible concentrations at each grid location

  - "kriging estimates present a serious drawback well known by geostatisticians as the smoothing effect in which small values are usually overestimated and large values underestimated… ... As a consequence of the smoothing effect ordinary kriging estimates do not reproduce either the histogram or the spatial variability as given by the semivariogram function." - Yamamoto, 2005

  - Kriged means/medians are not realistic concentration fields and should not be used to assess a Targeted Remedy

Overview of Applied Geostatistical Approaches

- ## Conditional simulation

    - Uses kriging distributions and the observed data to create random concentration fields

    - These fields reproduce the data distribution and spatial variability as defined by the semivariogram function; they are realistic concentration fields

    - Each random field is equally probable

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Steps in Implementing Conditional Simulation

I.   Segment the River

II.   Develop variograms

III. Krige

IV. Conditional Simulation

V.   Interpret Results

Segment the River

- Account for major features
  - Shoal and channel
  - Geomorphic features

- Try to preserve stationarity of concentration field (fixed mean)

River Segmentation – Upstream of RM 7.8

- Silt
  - Split into individual silt deposits

- Shoal/Channel
  - Split at gaps (i.e., where silt crosses the shoal/channel)
  - Split at EPA geomorphic breaks
  - Split at concentration pattern breaks

River Segmentation – Downstream of RM 7.8

- Shoal
  - Split at EPA geomorphic breaks

- Channel groupings
  - Bathymetry-based (RM 2.3-7.8)
  - Channel downstream of RM 2.3
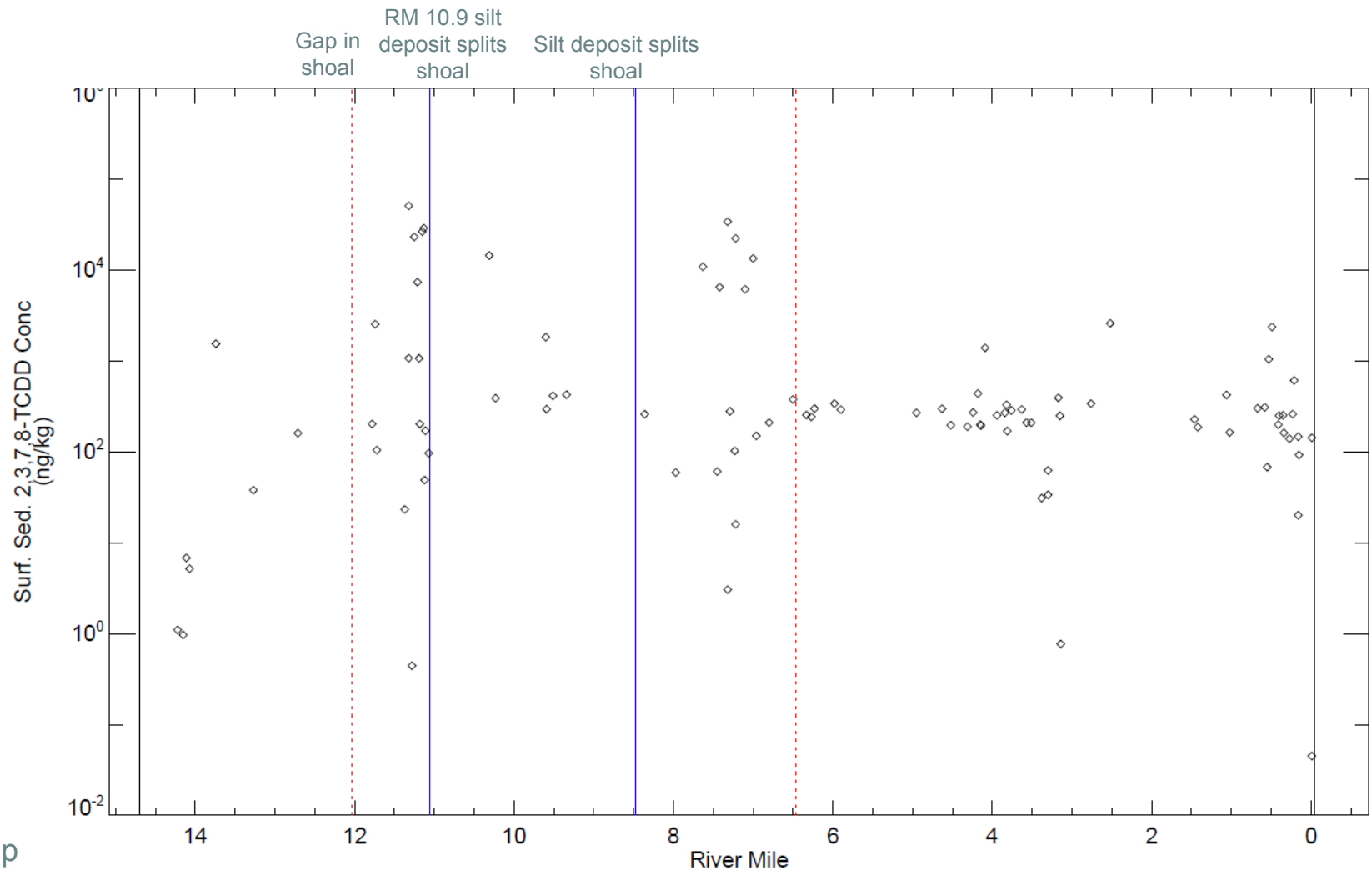 - No additional subdivisions within these groups
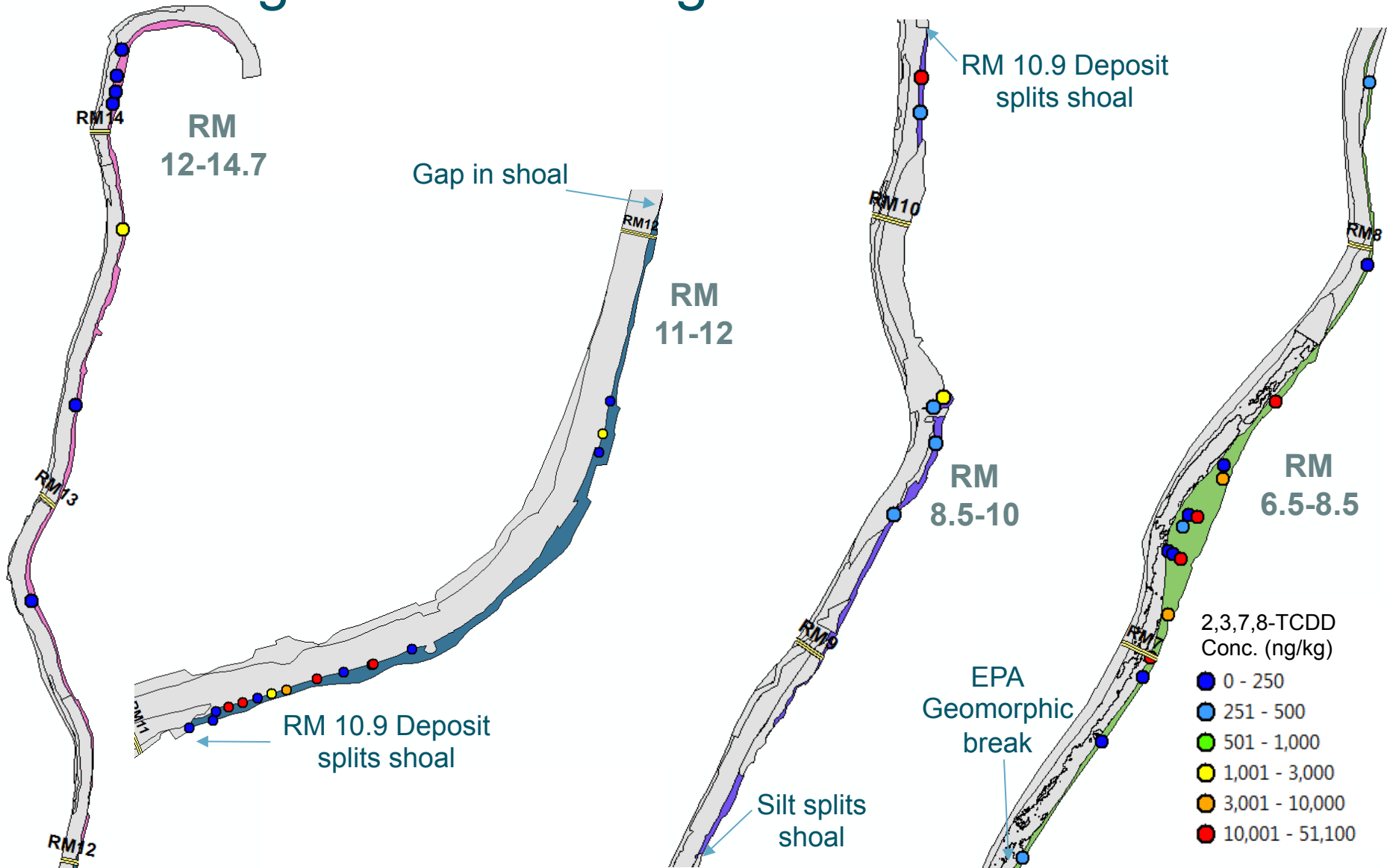
River Segmentation – Silt Upstream of RM 7.8

2,3,7,8-TCDD Conc. (ng/kg)

- 0 - 250
- 251 - 500
- 501 - 1,000
- 1,001 - 3,000
- 3,001 - 10,000
- 10,001 - 51,100

SI 6.2

SI 6.1

SI 7

SI 5

RM12

0   250   500
Feet

River Segmentation – Silt Upstream of RM 7.8

2,3,7,8-TCDD Conc. (ng/kg)

- 0 - 250
- 251 - 500
- 501 - 1,000
- 1,001 - 3,000
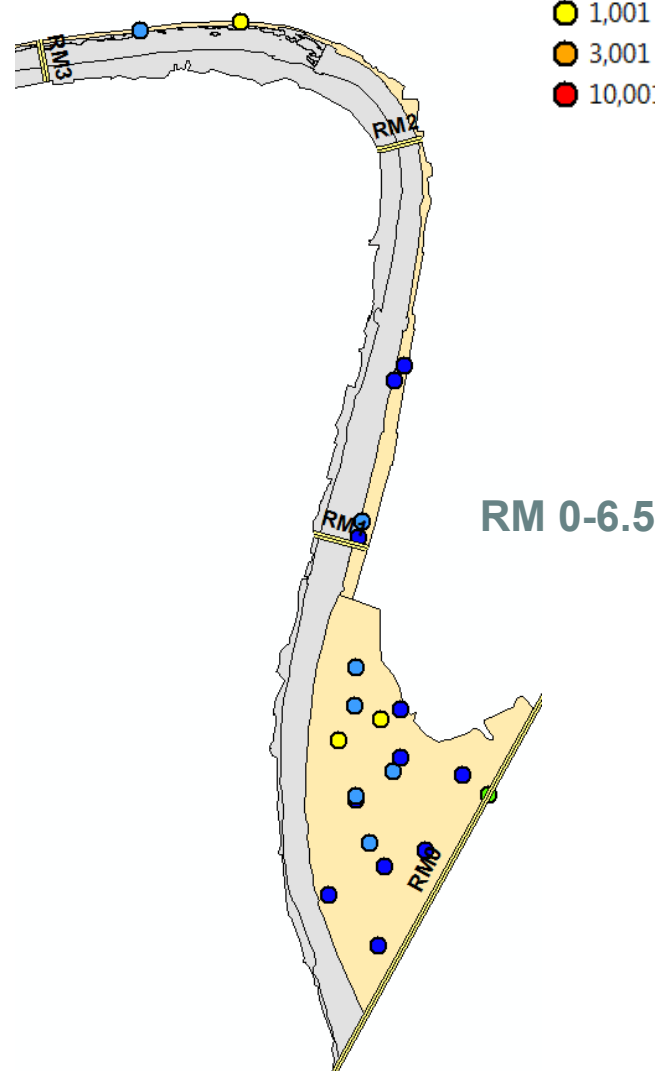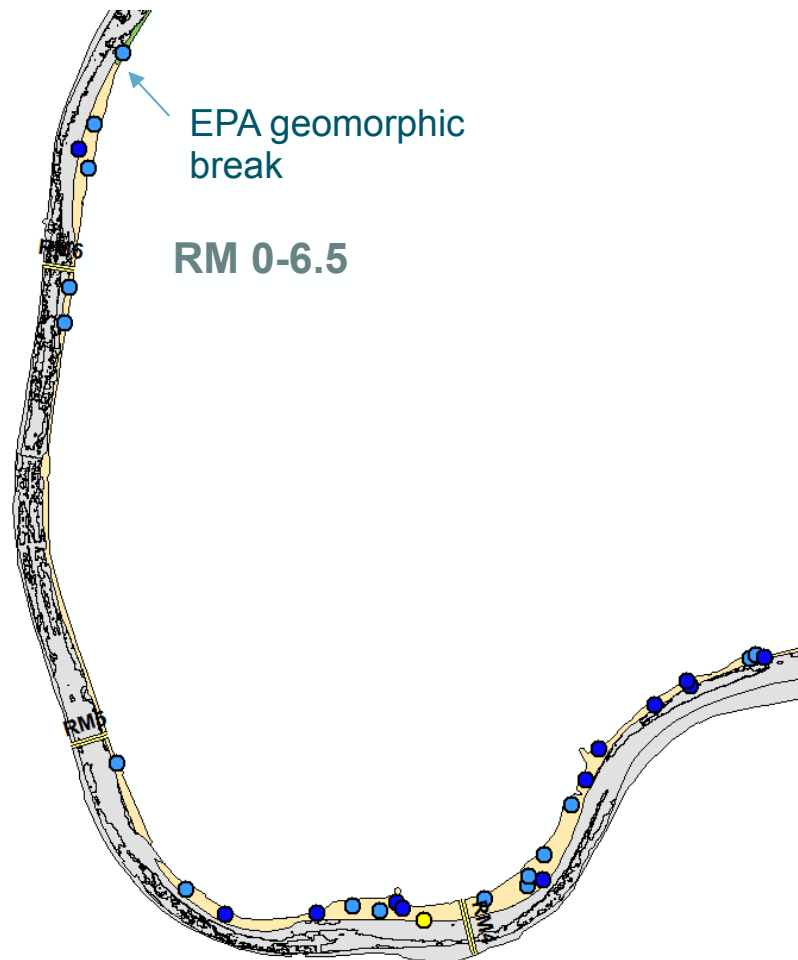- 3,001 - 10,000
- 10,001 - 51,100
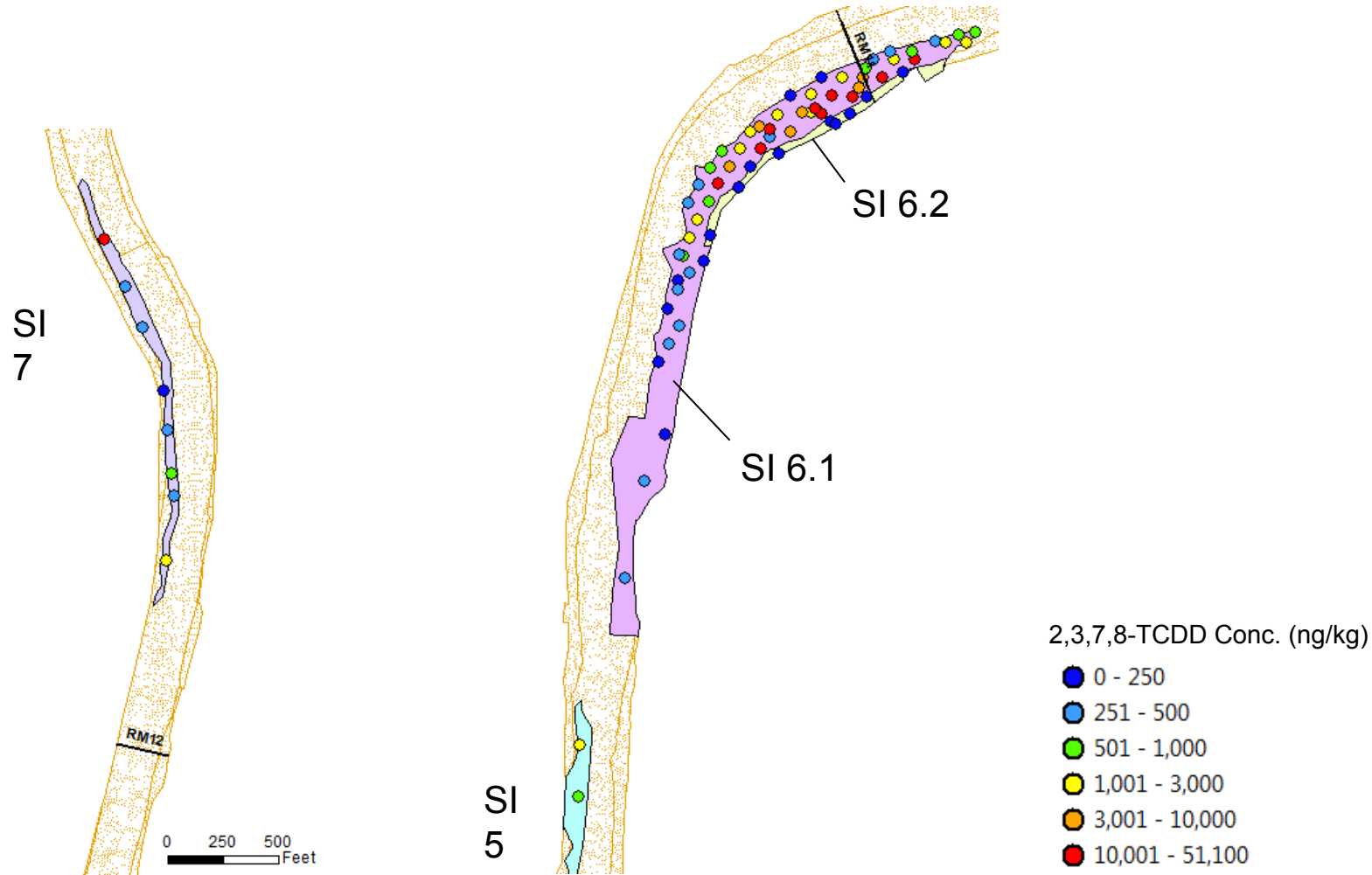
River Segmentation – Channel Upstream of RM 7.8

River Segmentation – Channel Upstream of RM 7.8

EPA geomorphic break

RM 14.7 – 13.75

EPA geomorphic break at bridge

RM 13.75 - 13

EPA geomorphic break at bridge

RM 13 – 12.5

RM 12.5 – 9.5

Silt splits channel

RM 9.5 – 7.8

2,3,7,8-TCDD Conc. (ng/kg)
- 0 - 250
- 251 - 500
- 501 - 1,000
- 1,001 - 3,000
- 3,001 - 10,000
- 10,001 - 51,100
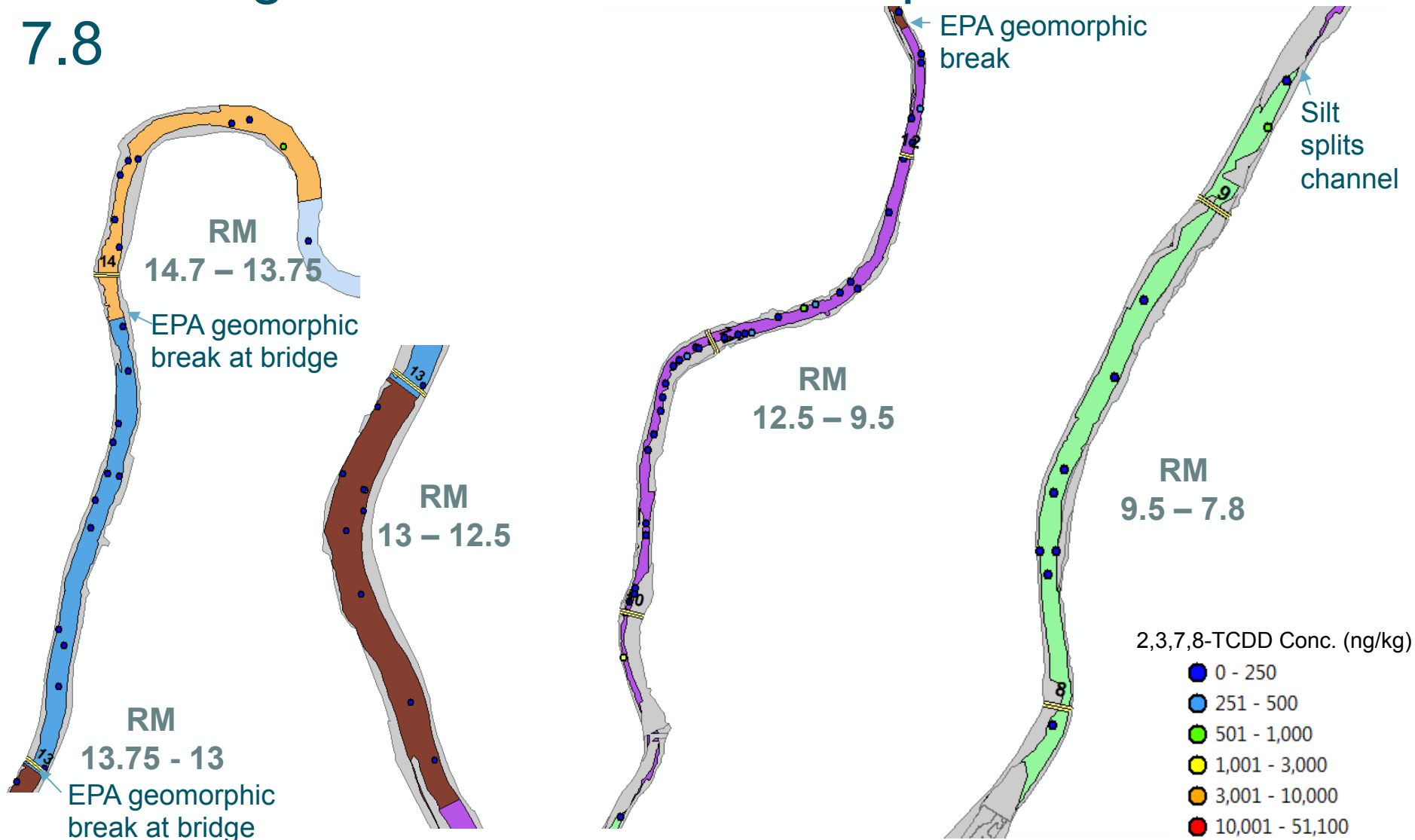
River Segmentation – Left Shoal
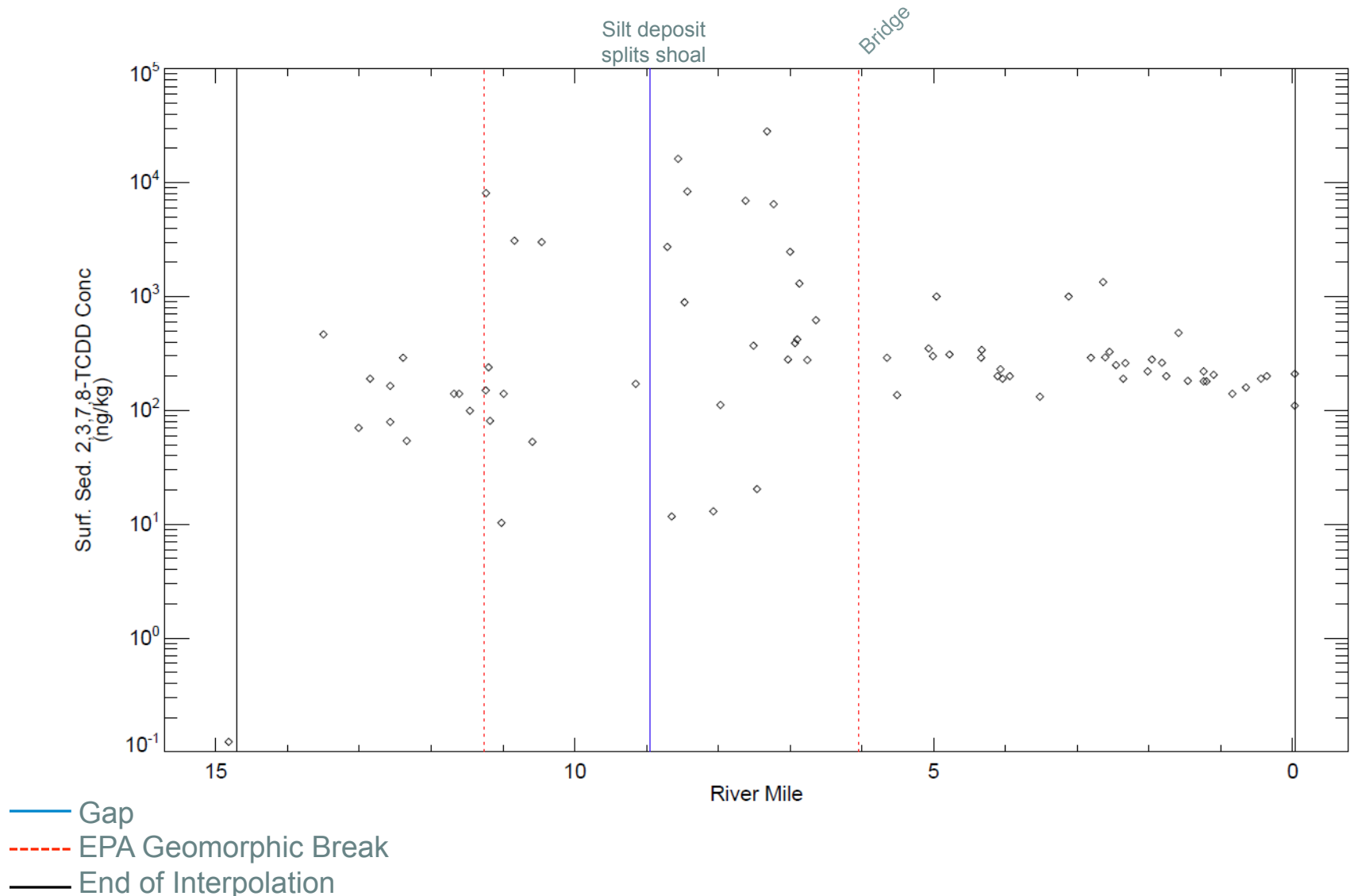
River Segmentation – Left Shoal

2,3,7,8-TCDD Conc. (ng/kg)
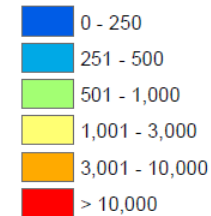
- 0 - 250
- 251 - 500
- 501 - 1,000
- 1,001 - 3,000
- 3,001 - 10,000
- 10,001 - 51,100

RM 14.5 – 11.5

RM 11.5 – 9

RM 9 - 6

RM 6 - 0

EPA geomorphic break

EPA geomorphic break at bridge

Silt splits shoal
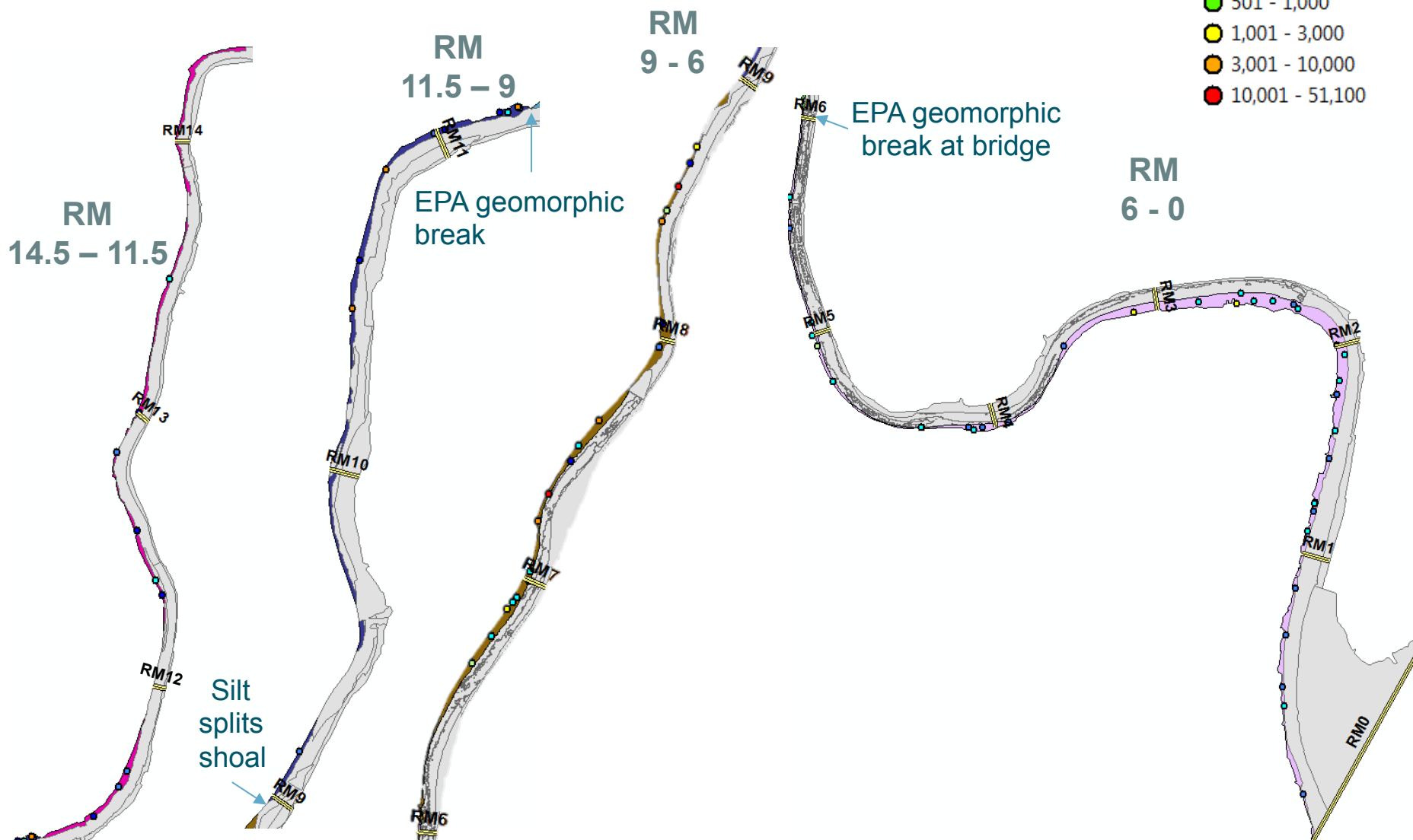
River Segmentation – Right Shoal

River Segmentation – Right Shoal

RM 12-14.7

Gap in shoal

RM 11-12

RM 10.9 Deposit splits shoal

RM 8.5-10

RM 10.9 Deposit splits shoal

EPA Geomorphic break

Silt splits shoal

RM 6.5-8.5

2,3,7,8-TCDD Conc. (ng/kg)
- 0 - 250
- 251 - 500
- 501 - 1,000
- 1,001 - 3,000
- 3,001 - 10,000
- 10,001 - 51,100

River Segmentation – Right Shoal

EPA geomorphic break

RM 0-6.5

RM 0-6.5

2,3,7,8-TCDD Conc. (ng/kg)
- 0 - 250
- 251 - 500
- 501 - 1,000
- 1,001 - 3,000
- 3,001 - 10,000
- 10,001 - 51,100

Approach to developing a variogram

- Assess need for directional variogram

- Transform data to obtain approximate normal distribution

  – At present, using log transformation; considering benefit of using normal scores transformation

- "Straighten" the river via a coordinate transform

- Bin data by separation distance and calculate semi-variance in each bin

- Model the relationship of semi-variance and separation distance

Spatial Correlation is Anisotropic – Greater Along Flow than Across Flow
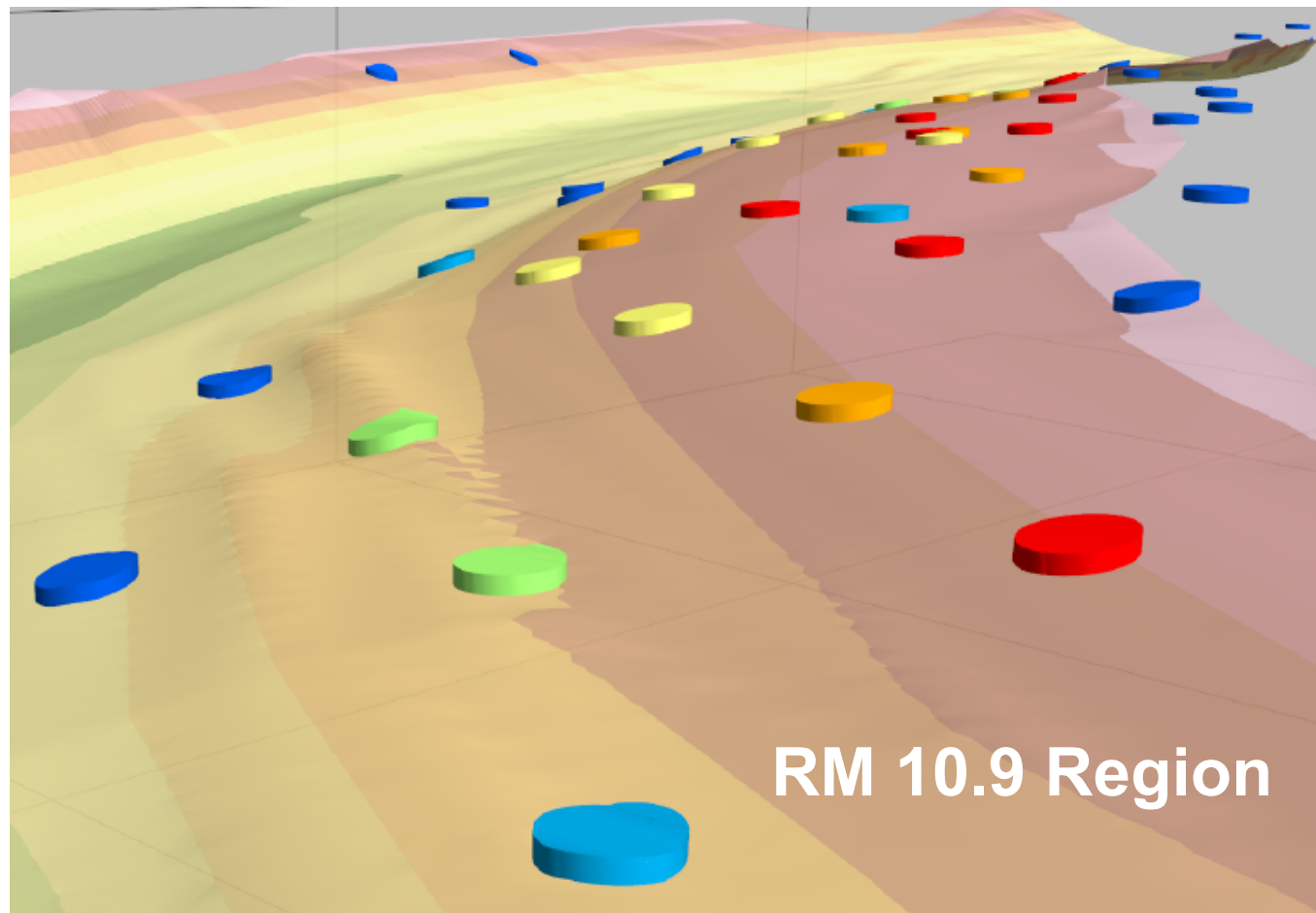
2,3,7,8-TCDD Concentrations (ng/kg)

Color	Range
■ (blue)	0 - 250
■ (cyan)	251 - 500
■ (green)	501 - 1,000
■ (yellow)	1,001 - 3,000
■ (orange)	3,001 - 10,000
■ (red)	> 10,000

2004 Bathymetry in feet (NGVD29)

Range	Range
2.1 - 4	-9.9 - -8
0.1 - 2	-11.9 - -10
-1.9 - 0	-13.9 - -12
-3.9 - -2	-15.9 - -14
-5.9 - -4	-17.8 - -16
-7.9 - -6	

RM 10.9 Region

Look Direction

0 250 500   1,000
Feet
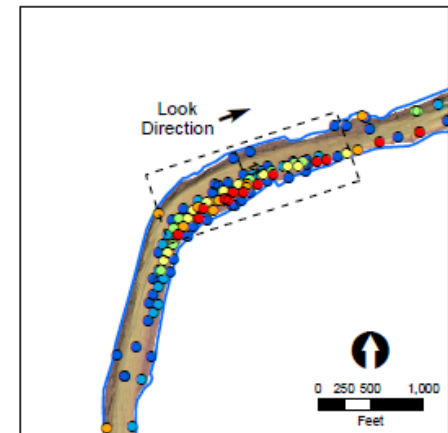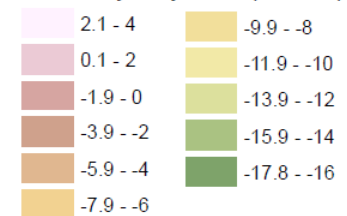
Vertical Exaggeration: 3X

Spatial Correlation is Anisotropic – Greater Along Flow than Across Flow

RM 7.5 Region

Approach used is to calculate along-flow variograms and assume anisotropy ratio to get cross-flow variograms. Ratio of 5 is used in work presented here.

Along-Flow 2,3,7,8-TCDD Variogram at RM 10.9
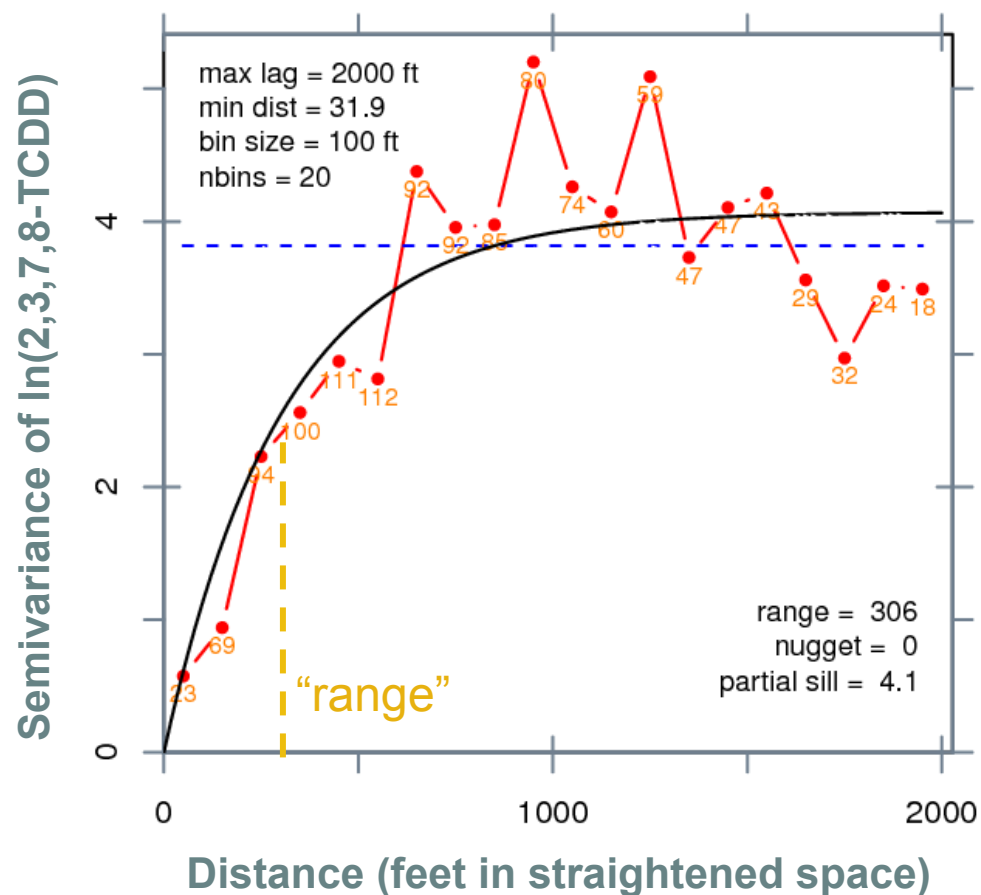
Range defined here as distance to 63% of sill (per GeoR convention)

Along-Flow Tetra-PCB Variogram at RM 10.9
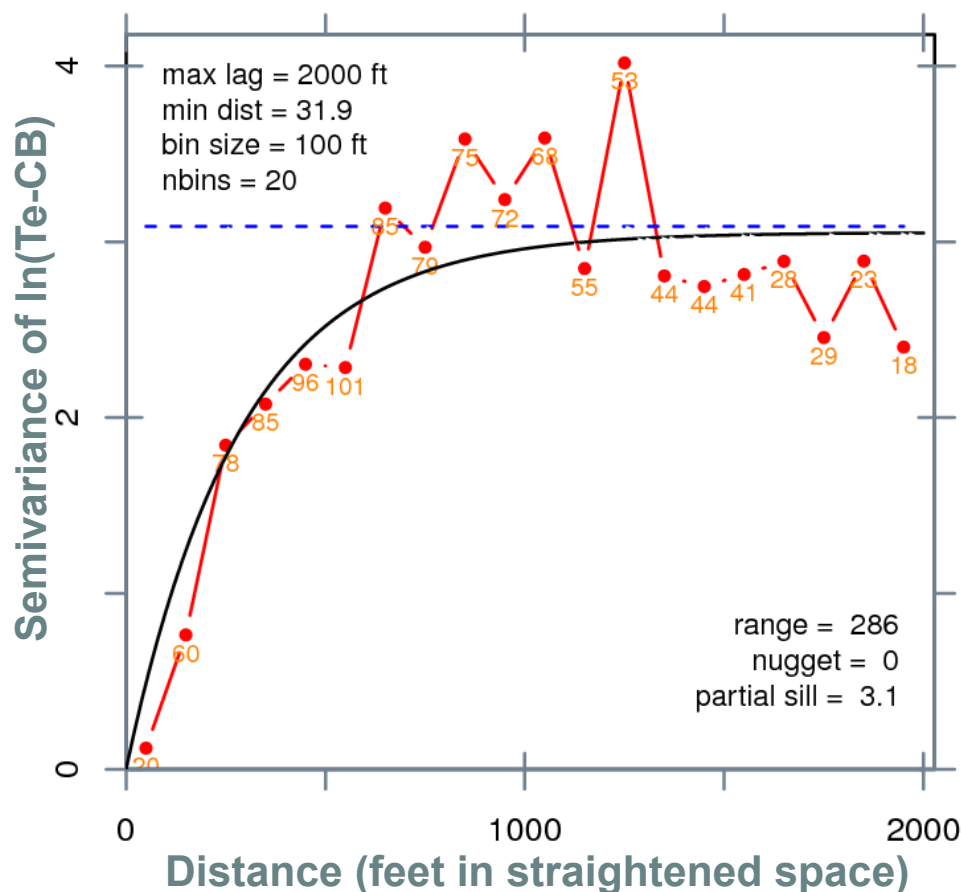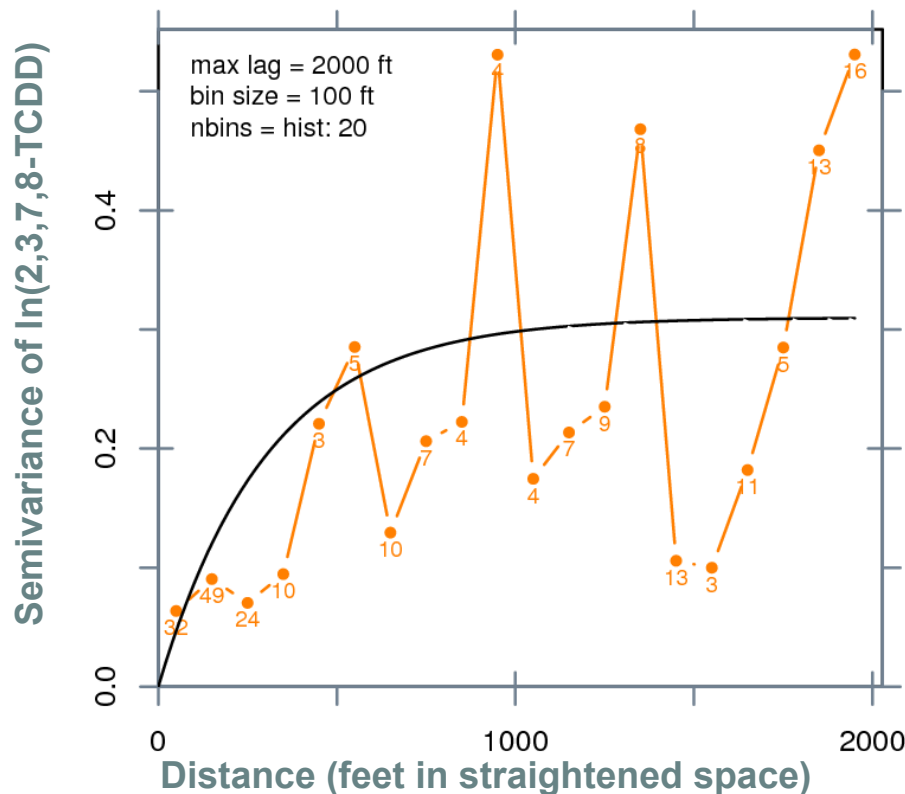

Similarity to 2,3,7,8-TCDD variogram supports understanding of spatial correlation

Variogram Model for Other Areas

- Insufficient data to develop individual variograms for other areas

- Assume same shape as RM 10.9, but local variance
  - Note: In results shown here, local variance reduced in two groups to eliminate excessive influence of data at tails of distribution (Right Shoal RM 0-6.5 and Channel RM 13.75-14.7)

Historical Data Support Applying RM 10.9 Variogram Shape to Other Areas

1995-2000 Data

Left Shoal RM 0-6

max lag = 2000 ft
bin size = 100 ft
nbins = hist: 20

Semivariance of ln(2,3,7,8-TCDD)

Distance (feet in straightened space)

Right Shoal RM 0-6.5

max lag = 2000 ft
bin size = 100 ft
nbins = hist: 20

Distance (feet in straightened space)
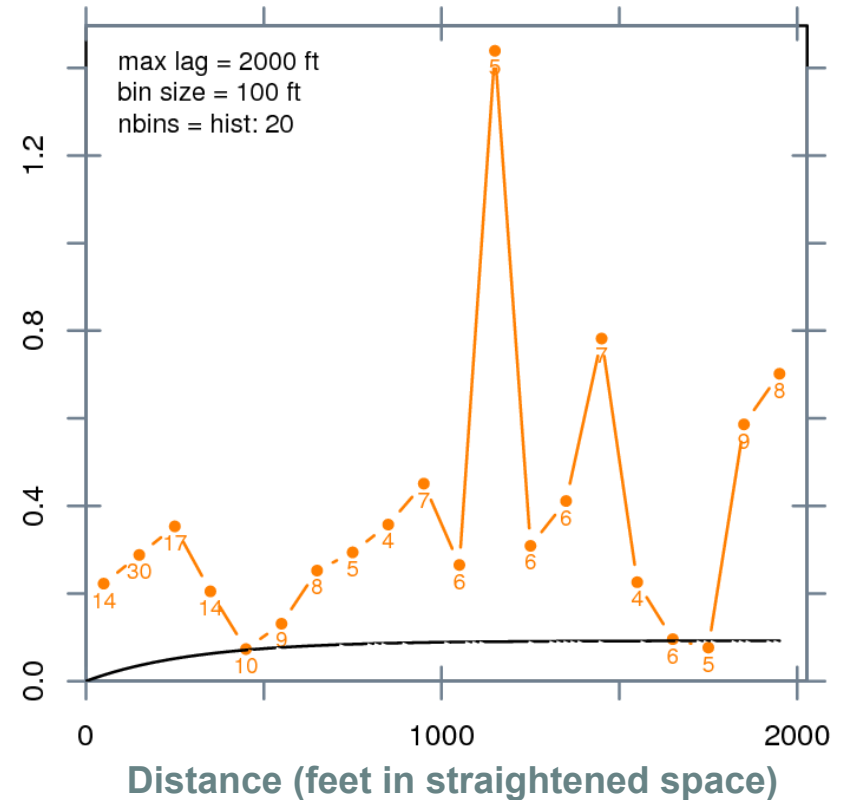
Phase 1 and Phase 2 Tierra Data Support Applying RM 10.9 Variogram Shape to Other Areas
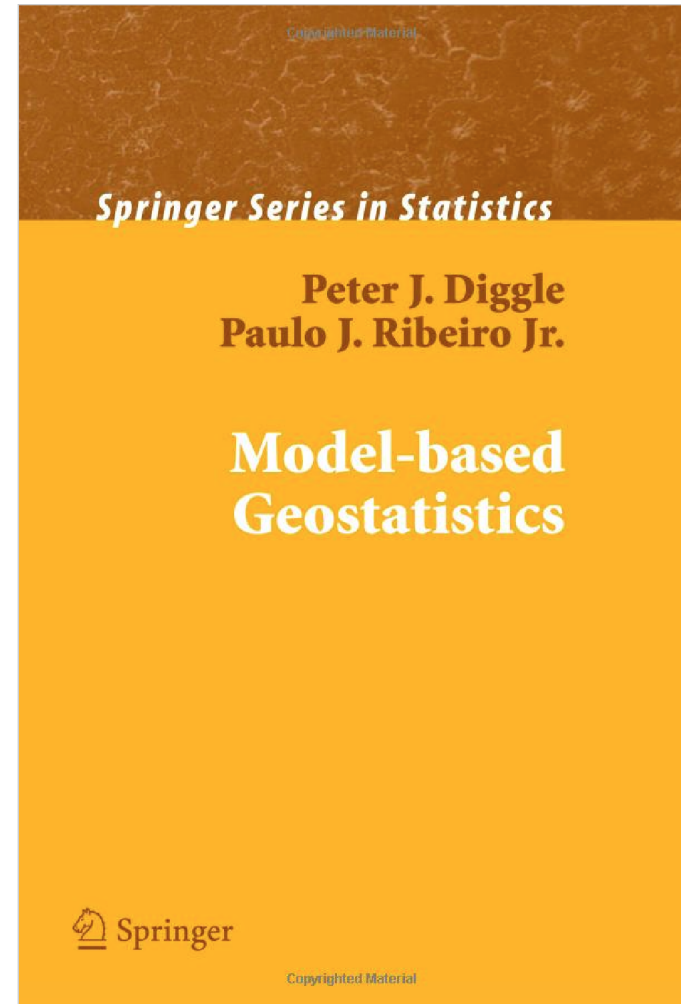
Phase 1&2 Data (0-2 ft segment)
Tolerance = +/- 10 degrees
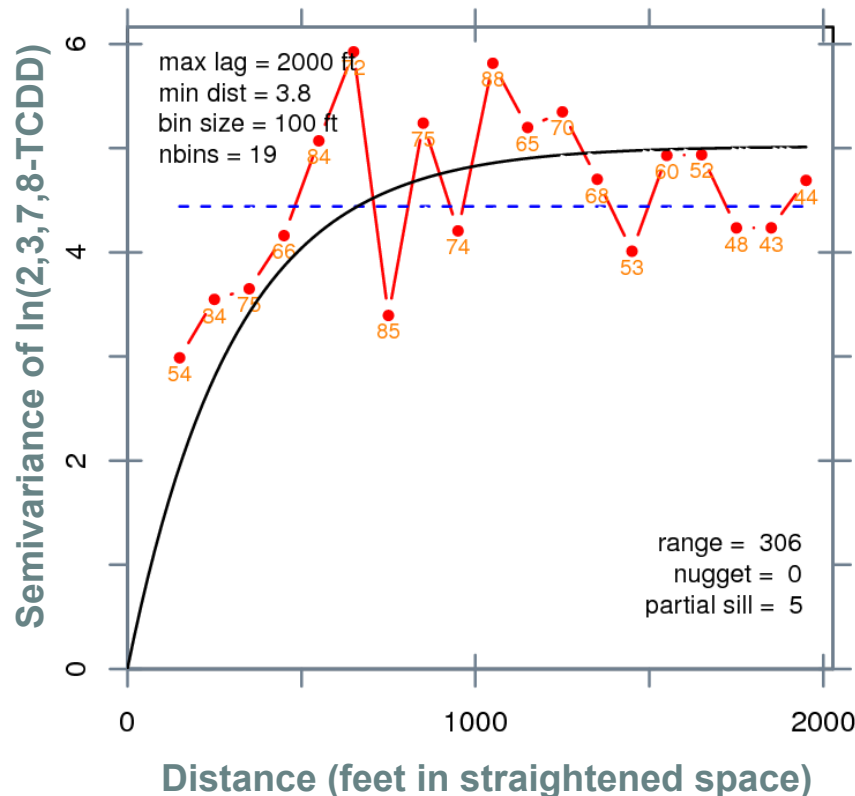
Comparison given less weight because of differing depth intervals and influence of ND data

Kriging Approach

- Simple Kriging in log space
  - Trends removed by group delineation
  - Simple Kriging was chosen over Ordinary Kriging to reduce complications with lagrange multipliers and conditional simulation
  - Simple vs Ordinary Kriging predictions were compared and were very similar

Conditional Simulation Software

- ## Two Choices in R platform
  - GeoR
    - Bayesian Approach
  - Gstat
    - Sequential Gaussian Simulation

- ## GeoR was chosen
  - Used for variogram analysis
  - More computationally efficient
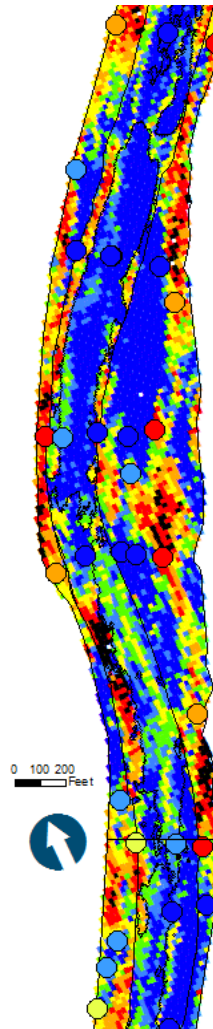 - Book supporting its use

Springer Series in Statistics

Peter J. Diggle
Paulo J. Ribeiro Jr.

Model-based Geostatistics

Springer

Preliminary Results– Map RM 7.5

Thiessen Mapping
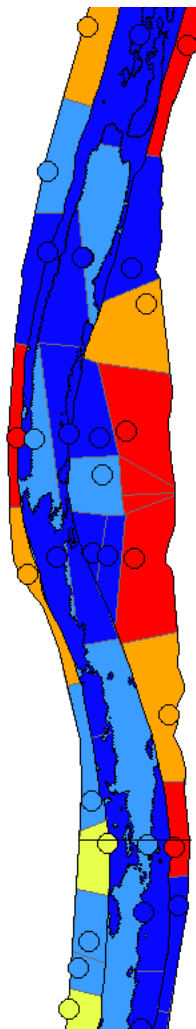
Kriging Median
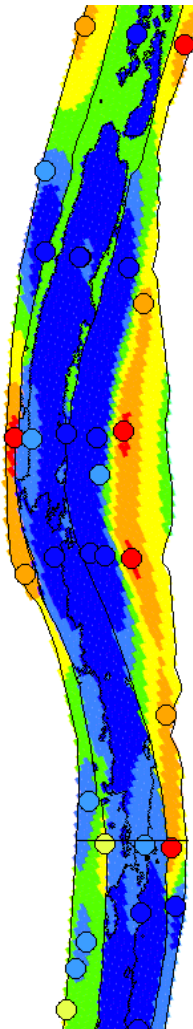
Kriging Variance
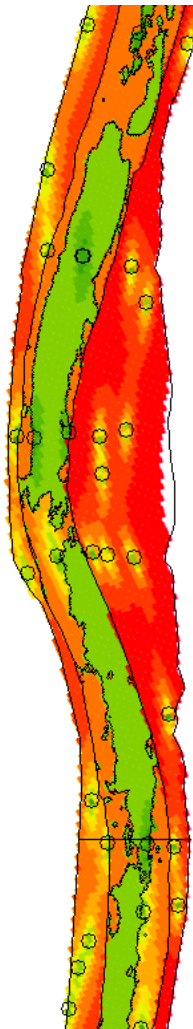
Conditional Simulation 1

⬤ Sample Location

— River Miles

▭ Interpolation Boundaries

2,3,7,8-TCDD Conc. (ng/kg)

■ 0 - 250
■ 251 - 500
■ 501 - 1,000
■ 1,001 - 3,000
■ 3,001 - 10,000
■ 10,001 - 51,100
■ 51,101 - 171,102

Kriging Variance (Natural Log)

■ 0.0 - 0.4
■ 0.5 - 0.8
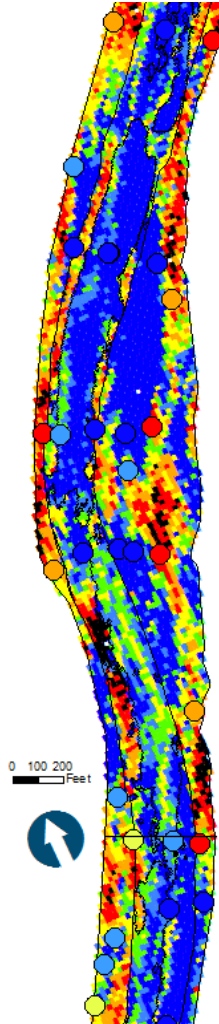■ 0.9 - 1.2
■ 1.3 - 1.7
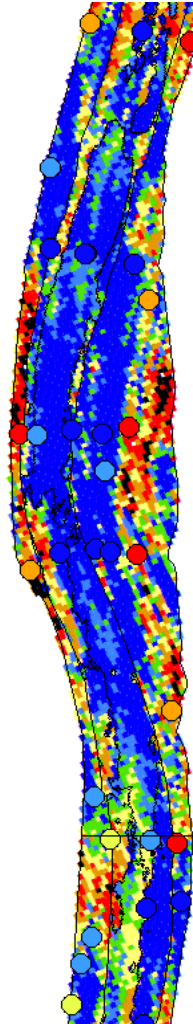■ 1.8 - 2.3
■ 2.4 - 2.9
■ 3.0 - 3.7
■ 3.8 - 4.7
■ 4.8 - 6.3
■ 6.4 - 8.3

0 100 200
Feet

Preliminary Results– Conditional Simulations
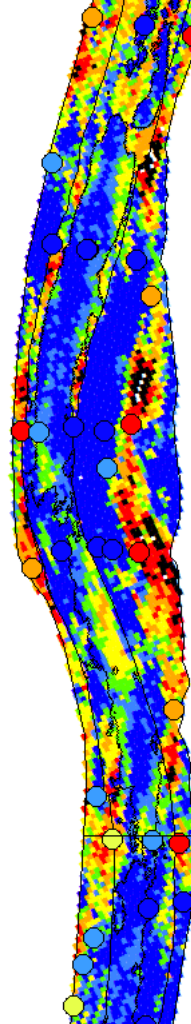

Conditional Simulation 1

Conditional Simulation 2

Conditional Simulation 3

Legend:
- Sample Location
- River Miles
- Interpolation Boundaries

2,3,7,8-TCDD Conc. (ng/kg)
- 0 - 250
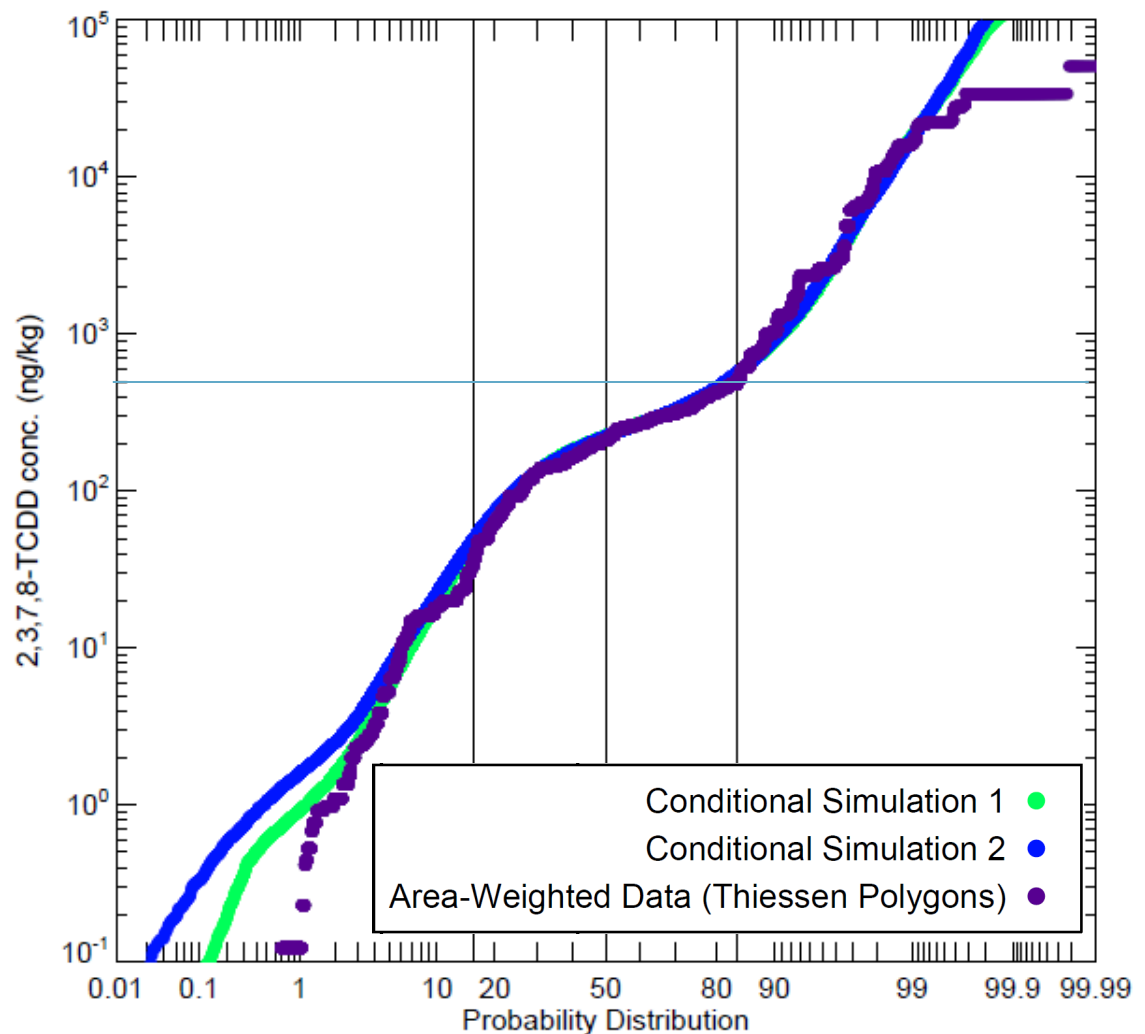- 251 - 500
- 501 - 1,000
- 1,001 - 3,000
- 3,001 - 10,000
- 10,0001 - 51,100
- > 51,100
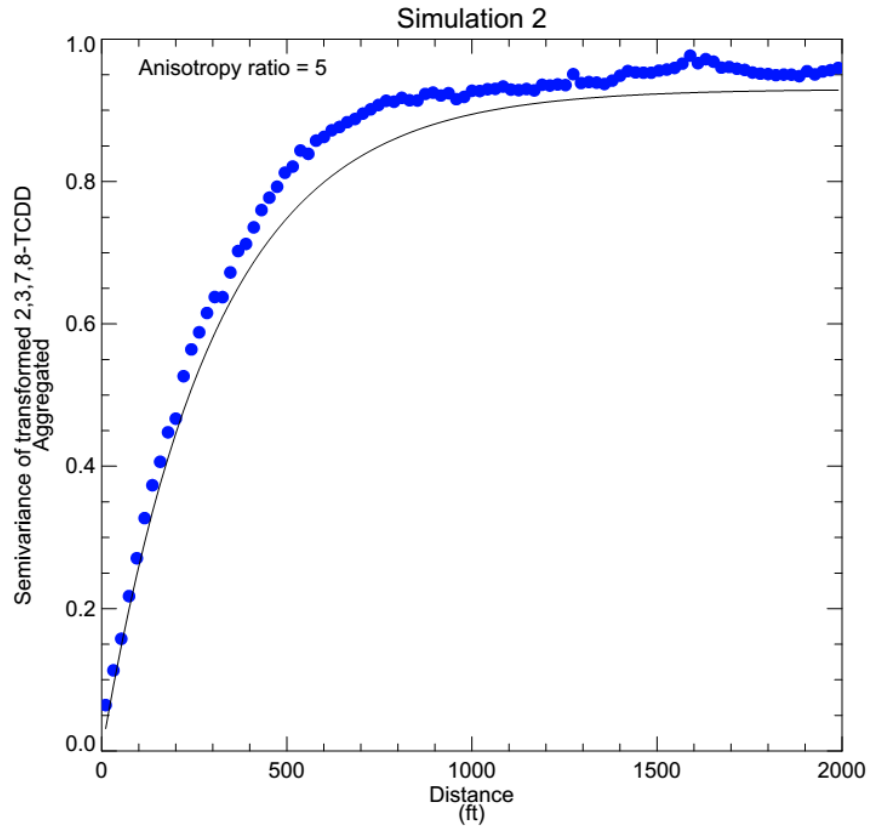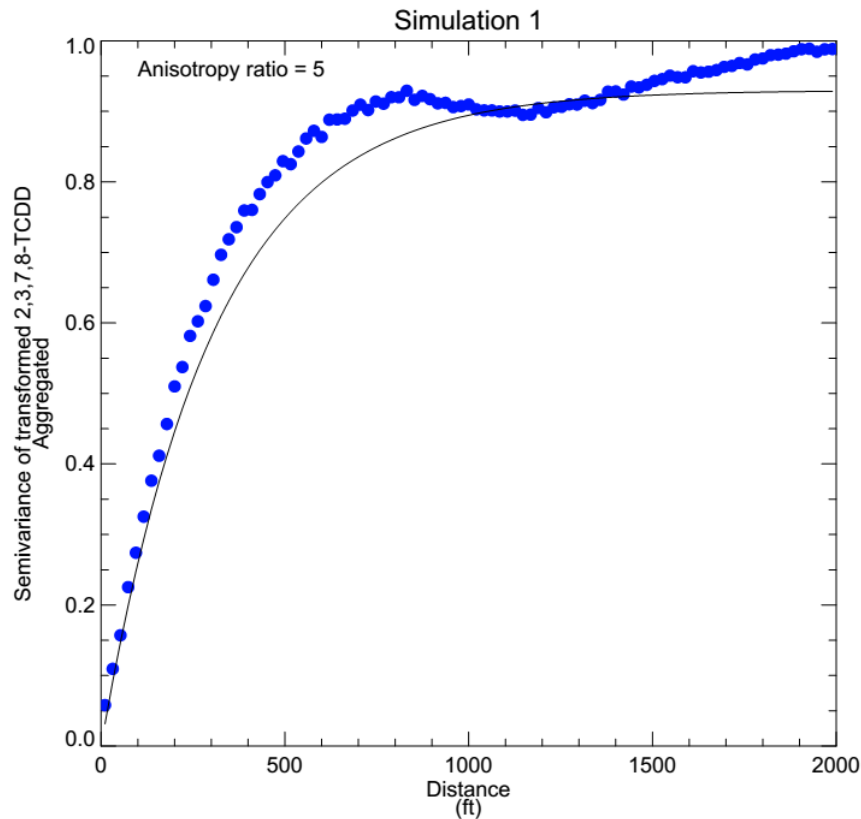
QC of Results - Concentration Distributions

- CS recovers the concentration distributions

- Comparison to Area-Weighted Data

QC of Results – Aggregate Variogram

- ## CS recovers the variogram

Note: Does not include Right Shoal RM 0-6.5 and Channel RM 13.75-14.7
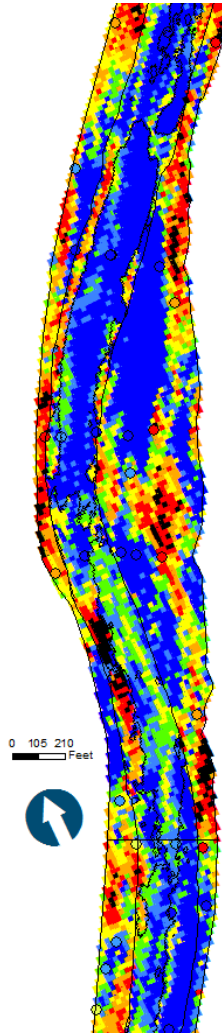
Treatment of Simulation Results for Crafting a Targeted Remedy Alternative
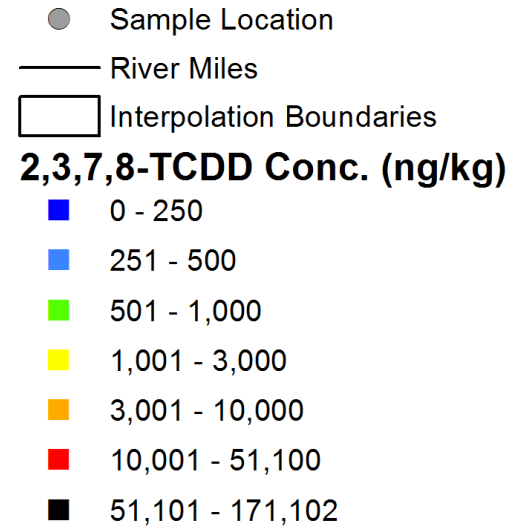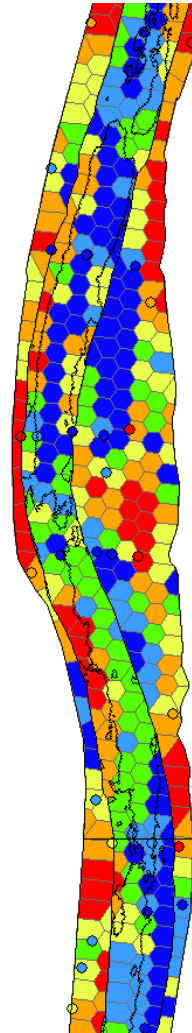
- Average results at 80-ft scale
  - Used as estimate of smallest remedial unit

- Cap concentrations at max. observed (51,100 ng/kg)
  - Occasional prediction of unrealistically high concentrations biases estimate of benefit achieved by targeted remediation

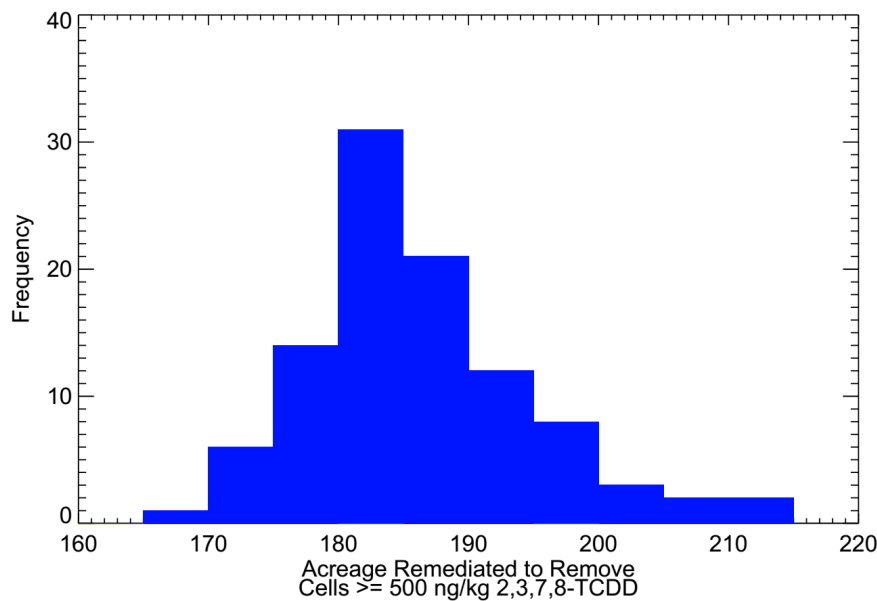# Example of Proposed FS Approach (RM 7.5)

Conditional Simulation 1

Conditional Simulation 1 Averaged on 80-ft grid decision units
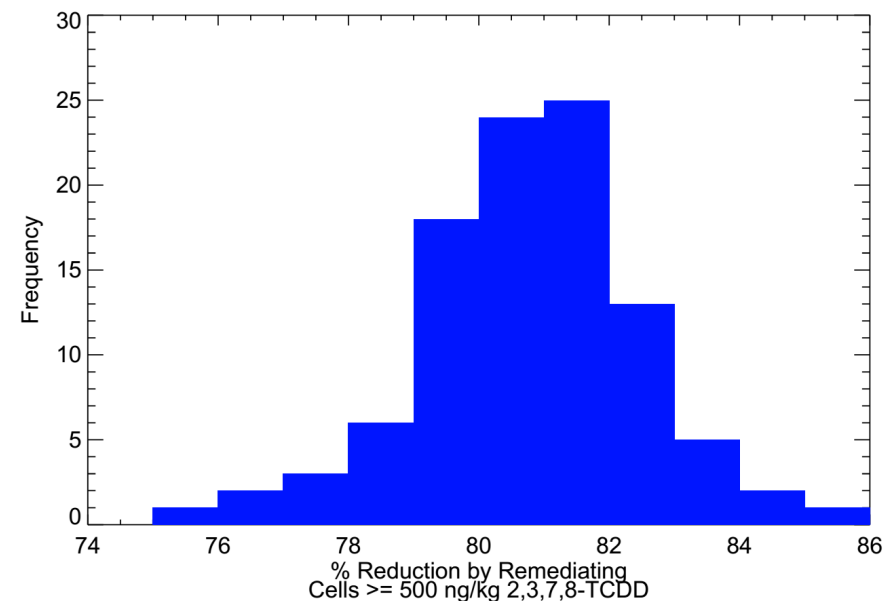
Legend:
- ● Sample Location
- — River Miles
- ▢ Interpolation Boundaries

2,3,7,8-TCDD Conc. (ng/kg)
- 🟦 0 - 250
- 🟦 251 - 500
- 🟩 501 - 1,000
- 🟨 1,001 - 3,000
- 🟧 3,001 - 10,000
- 🟥 10,001 - 51,100
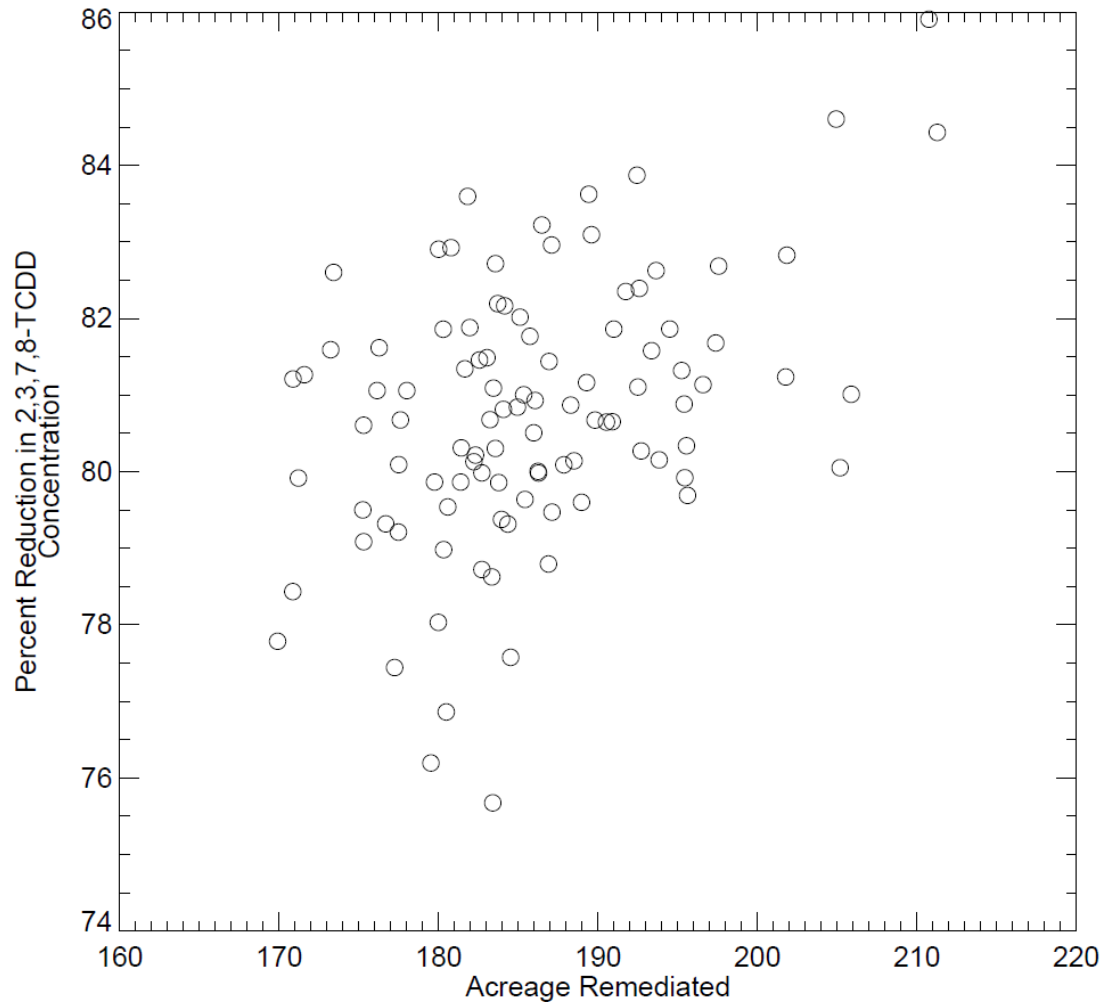- ⬛ 51,101 - 171,102

Histograms – RAL 500 ng/kg

Acres Remediated

% Reduction

Percent Reduction vs Acreage: 500 ng/kg RAL

Summary

- Conditional simulation provides a means to quantify mapping uncertainty

- It provides information that can be used to make informed decisions that account for uncertainty

  – Choosing an RAL

  – Choosing areas meeting an RAL

  – Crafting a design sampling program aimed at efficiently reducing uncertainty

- Mapping using the LPR RI data set provides understanding sufficient to craft remedial alternatives for an FS

  – Uncertainty is reasonable and can be reduced during remedial design

Backup Slides

Effect of Trimming Tails of the Right Shoal RM 0-6.5 Sample Data on the Variogram and its Comparison to Historical Data

Variogram model after trimming

Variogram model before trimming